

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 122 °C

Global applicability domain: Inside

Local applicability domain index: 6.56e-01

Confidence level: 8.50e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Chloroethanol</div> <div>Measured: 129</div> <div>Predicted: 122</div>	<div>Image not found</div> <div>Ethyl hydroperoxide</div> <div>Measured: 95.0</div> <div>Predicted: 99.9</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 97.2</div> <div>Predicted: 96.5</div>
<div>Image not found</div> <div>2-Methoxyethanol</div> <div>Measured: 124</div> <div>Predicted: 123</div>	<div>Image not found</div> <div>2-Chloropropan-1-ol</div> <div>Measured: 134</div> <div>Predicted: 137</div>	